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14. ABSTRACT The primary goals of this research proposal consist of the development of mathematical tools for high performance materials. The microstructure of these complex fluids consists of macromolecules whose shape, conformation, and rigidity/flexibility interact with the flow to effect molecular scare alignment that controls the ultimate performance properties of the solid material. Our approach has focused on mesoscale, moment-averaged theories derived for liquid crystalline polymer (LCP) materials. We aim for:

- modeling and simulation of free surface fiber processes for anisotropic, viscoelastic materials;
- exact constructions of the patterns that are routinely observed in experiments, and for which no mathematical descriptions were available;
- for fundamental understanding of nematic dynamics and phase transitions, and of the response of these complex fluids to flows that approximate finer and film processes;
- and, for development of numerical codes to resolve the interactions between microstructure and flow.

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Final Progress Report

FIBER FLOWS AND TECHNOLOGICAL APPLICATIONS

AFOSR Contract F49620-97-1-0001

Principal Investigator: M. Gregory Forest
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Objectives

The primary goals of this research proposal consist of the development of mathematical tools for high performance materials. The microstructure of these complex fluids consists of macromolecules whose shape, conformation, and rigidity/flexibility interact with the flow to effect molecular scale alignment that controls the ultimate performance properties of the solid material. Our approach has focused on mesoscale, moment-averaged theories derived for liquid crystalline polymer (LCP) materials. We aim for:

- modeling and simulation of free surface fiber processes for anisotropic, viscoelastic materials;
- exact constructions of the patterns that are routinely observed in experiments, and for which no mathematical descriptions were available;
- for fundamental understanding of nematic dynamics and phase transitions, and of the response of these complex fluids to flows that approximate fiber and film processes;
- and, for development of numerical codes to resolve the interactions between microstructure and flow.

Status of Effort

- Our models for thermotropic liquid crystalline fiber spinning processes are in use today in manufacturing plants of Hoechst Celanese Corporation; recent publications document the academic contributions ([1],[3], [8], [13], [11], [9]).
- We have used a full tensor description of flowing nematic LCPs to identify new phenomena associated to the classical isotropic-to-nematic

phase transition, namely, the participation of director instabilities in the transition. Previous analyses have only studied order parameters. This discovery then leads to analogous phenomena in flow-driven transitions. ([14], [12], [15])

- We have constructed exact defect structures, in terms of geometric core defects, in response to an imposed planar elongational flow ([12]).

Accomplishments

- We have provided a rigorous study of the interaction between microstructure and free surface filament flows, deriving asymptotic models ([1],[3]) and explaining the suppression of capillary instability by anistropic viscoelasticity ([6],[7]).

- With regard to LCP processing, we have developed the first comprehensive model for thermotropic liquid crystal polymer fibers. In [13], we: assemble the important physics; derive the equations; replace the standard two phase model by a phase field model for liquid to solid phase transition; calculate processing steady states (of a two point boundary value problem); develop a linearized stability analysis and numerical code; then apply the codes to study fiber behavior and stability.

- In [11], we apply the thermotropic LCP spin model and code to deduce fiber performance properties, process sensitivity, and bound on spinning speed due to heat loss, air drag, temperature conditions in the spinline, and the material properties of LCPs.

- In [10], we show the original Doi model for flows of liquid crystal polymers is not well-posed at low concentrations. We then show how to regularize the equations with a variety of physical effects.

- In [9], we couple crystallization kinetics to isothermal models for LCP fibers. This is the first model that resolves orientation-induced crystallization, with a coupled order parameter dynamics.

- In [14], we use a full tensor description of nematic LCPs and rigorously analyze the Doi type kinetic theory models which incorporate short range excluded volume and intermediate range elasticity potentials. We

deduce all homogeneous patterns, their stability, and phase transitions; this work revises the classical explanation of the isotropic to nematic phase transition. We then proceed to derive exact banded patterns which are routinely observed in experiments. These patterns can be induced by order parameter variations and by sinuous optical axes.

- In [12], we study imposed elongational flows of LCPs and derive exact, closed form solutions of the flow/orientation equations which correspond to core defects. These defects have a logarithmic pressure singularity along the axis of symmetry of the flow.

- In [15], we deduce all homogeneous equilibrium patterns, their stability, and all phase transitions of LCPs in imposed elongational flows. We identify both order parameter and director instabilities, which were not recognized previously. We predict that only uniaxial patterns are stable in axial elongation, whereas in planar elongation beyond a very low LCP concentration the only stable patterns are fully biaxial.

Personnel Supported

The PI has been supported through summer salary and travel. Postdocs Hong Zhou and Dan Anderson have been supported through partial academic year support and travel.

Transitions

- The AFOSR contract has provided the basis for a long term collaboration with Hoechst Celanese Corporation in the modeling of textile fibers. Our models and codes are in use internationally on the manufacturing floor. This relationship has terminated due to a shift in emphasis by the parent company; most of the group we worked with is now departed.

- A secondary, developing relationship made possible by this research involves the transition of our thermal fiber capability to Corning, Inc. for their manufacture of optical fibers.

- The PI has begun discussions with scientists at Wright Patterson AFB, Materials Directorate, Dayton, OH, in research toward understanding

various phenomena related to laser hardened materials and organic polymers.

Interactions

Invited lectures at meetings, conferences, and colloquia have resulted from this supported research. A selected list since 1999 is:

- Workshop on Multicomponent and Multiphase Fluid Dynamics, U. Penn, invited address, March, 1999.
- MSRI Workshop on Self Assembling Geometric Structures in Material Science, invited address, April, 1999.
- IMACS International Conference on Nonlinear Evolution Equations and Wave Phenomena, plenary address, University of Georgia, April, 1999.
- SIAM Workshop on Dynamical Systems, plenary address, Snowbird, UT, May, 1999.
- Society of Rheology Annual Meeting, Madison, WI, October 9, 1999.
- Workshop on Integration of Integrability into Science and Mathematics, in honor of V. Zakharov, Tucson, AZ, October 30, 1999.
- University of California-Irvine Colloquium, Irvine, CA, March 13, 2000.
- Southeastern Regional Meeting of the American Mathematical Society, Lafayette, LA, April 15, 2000.
- Materials Research Society Spring Meeting, Symposium on Multiscale Modeling of Organic Materials, San Francisco, CA, April 25, 2000.
- SIAM Materials Science Meeting, Philadelphia, PA, May 24, 2000.
- Center for Advanced Scientific Computation, Lawrence Livermore National Laboratory, June 27, 2000.

- Air Force Office of Scientific Research Grantees' and Contractors Meeting, Stanford University, June 29, 2000.

Honors/Awards None.

Publications (listed below in REFERENCES format)

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[9] An isothermal model for high speed spinning of liquid crystalline polymer fibers–Coupling of flow, orientation, and crystallization, (with T. Ueda), Journal of Non Newtonian Fluid Mechanics 84, 109-121 (1999).

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[12] Nonhomogeneous patterns with core defects in elongational flows of liquid crystal polymers, (with Q. Wang and H. Zhou), J. Rheology 43(6), 1573-1582, (1999).

[13] Thermotropic liquid crystalline polymer fibers, (with Hong Zhou and Qi Wang), SIAM J. Appl. Math. 60(4), 1177-1204 (2000).

[14] On phase transitions and pattern formation in nematic liquid crystal polymers, (with Q. Wang and H. Zhou), Physical Review E 61(6), 6665-6662, (2000).

[15] Homogeneous pattern selection and director instabilities of nematic liquid crystal polymers induced by elongational flows, (with Q. Wang and H. Zhou), Physics of Fluids 12(3), 490-498, (2000).